Exceptional service in the national interest

Sandia National Laboratories

Charon Overview

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Staffing and Funding

Sandia National Laboratories

- Personnel
  - 1355
    - Larry Musson
    - Gary Hennigan
    - Suzey Gao
    - Mihai Negoita
    - Andy Huang
    - Jason Gates
    - Joe Castro
- Funding
  - ASC/IC
  - ASC/P&EM
  - ASC/V&V

What is Charon?

- Semiconductor *TCAD* code with support for modeling displacement damage due to neutron radiation as well as effects from other sources of radiation (e.g. ionization)
- Finite-volume and finite-element discretizations of governing PDEs
  - Drift-Diffusion
  - Drift-Diffusion + Energy (Lattice Heating)

Electric Potential

$$\nabla \cdot \left(\epsilon \vec{\mathbf{E}}\right) = q\left(p - n + C\right)$$
$$\vec{\mathbf{E}} = -\nabla V$$

Constitutive Relations

$$\vec{\mathbf{J}}_n = q\left(n\mu_n \vec{\mathbf{E}} + D_n \nabla n\right)$$
$$\vec{\mathbf{J}}_p = q\left(p\mu_p \vec{\mathbf{E}} - D_p \nabla p\right)$$

Conservation

$$\nabla \cdot \vec{\mathbf{J}}_n - qR = q\frac{\partial n}{\partial t}$$
$$-\nabla \cdot \vec{\mathbf{J}}_p - qR = q\frac{\partial p}{\partial t}$$

Lattice Heating

$$\nabla \cdot \left(\kappa \nabla T_L\right) + H = \rho c \frac{\partial T_L}{\partial T}$$

Unique Capabilities Provided by Charon

- Two & three dimensional + parallel capability
- Production quality code using current best practices for software development
  - Adheres to formal SQE practices
    - Monitored with periodic audits
  - Utilizes rigorous verification
    - MMS (Method of Manufactured Solutions)
    - Automated regression testing (nightly/weekly)
- Utilizes latest solver technology
  - Via solvers in Sandia's Trilinos toolkit
- Incorporates empirical (fast running) and high fidelity physics models for displacement damage

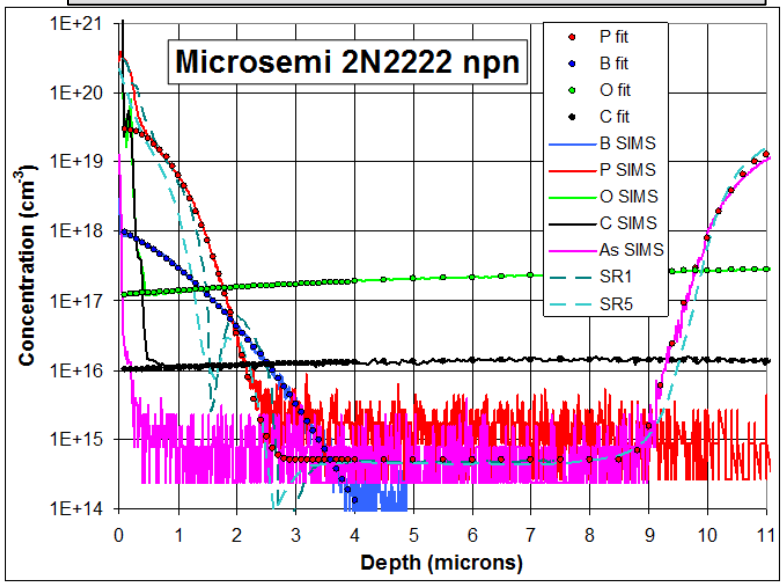
Environments & Device Modeling Capability

Sandia National Laboratories

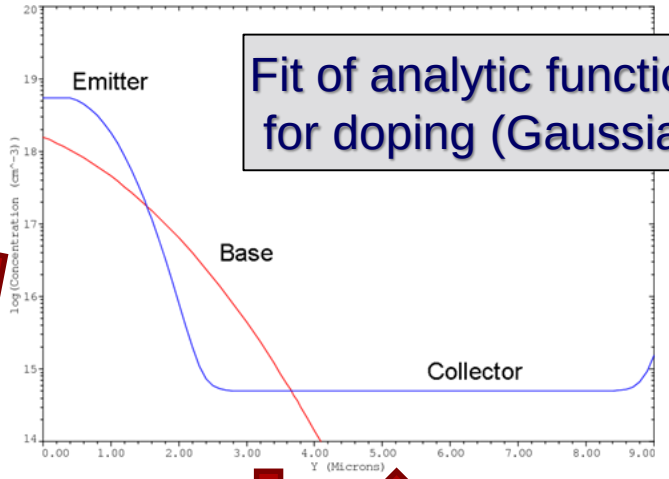
- Environments
  - Normal
  - Dose Rate – reactor environments
  - Total Dose – not validated
  - SEE – Some early, limited capability
- Devices
  - Diodes
  - BJT (Si)
  - HBT (III-V)
  - FETs
  - Memristor
  - Ultra-Wide Band Gap Diodes (new models)

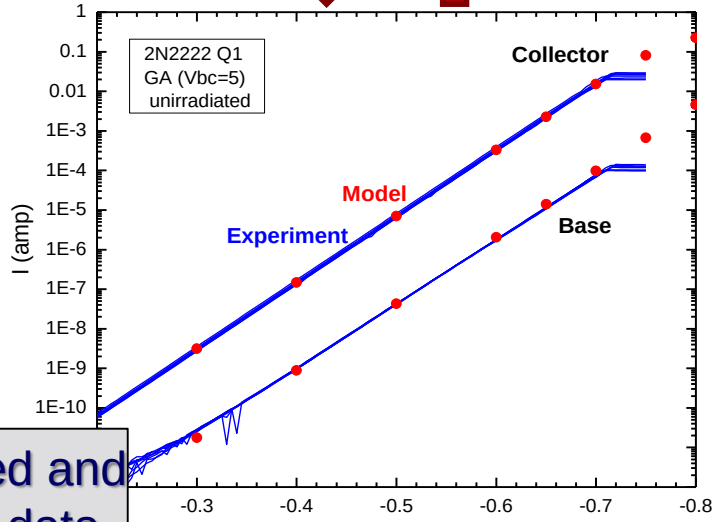
Normal Environment Characterization (COTS BJT Example)

SIMS and SR dopant and impurity concentration measurements



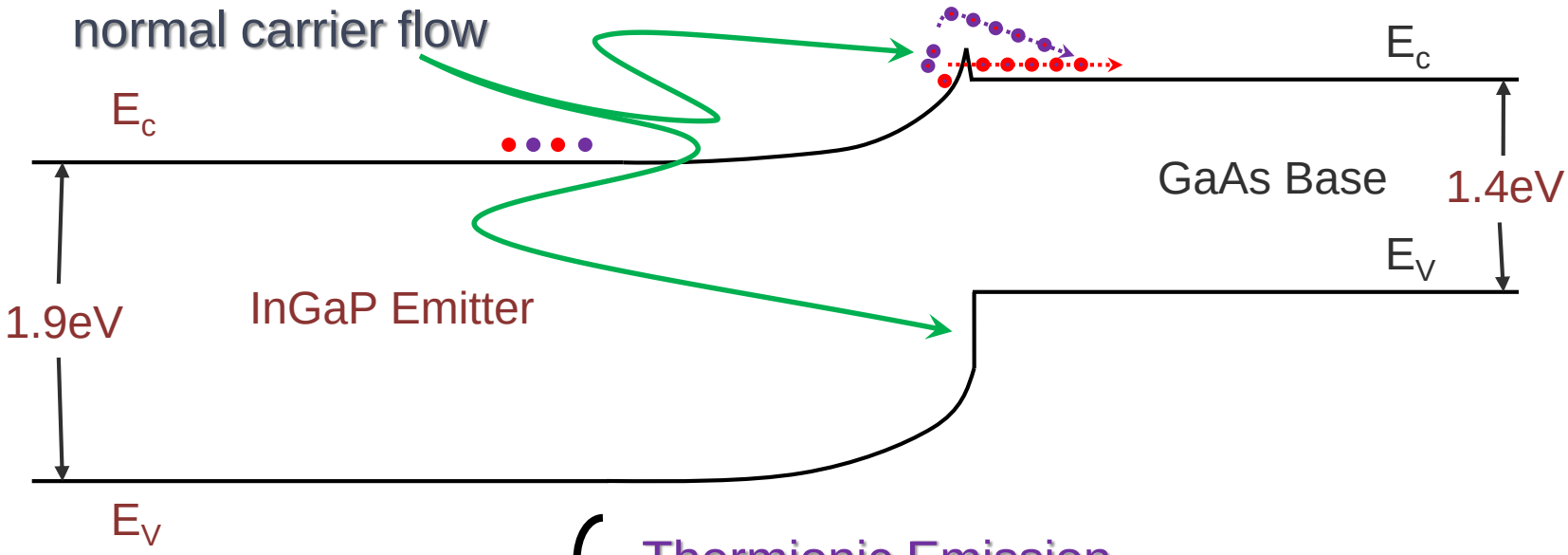
Fit of analytic functions for doping (Gaussian)





Comparison of computed and experimental Gummel data

Bandgap in a Np^+ Heterojunction



There are two other mechanisms however that will allow carrier transport:

Thermionic Emission

- Carriers receive enough energy via thermal processes to overcome the barrier

Tunneling

- Carriers may tunnel through the barrier

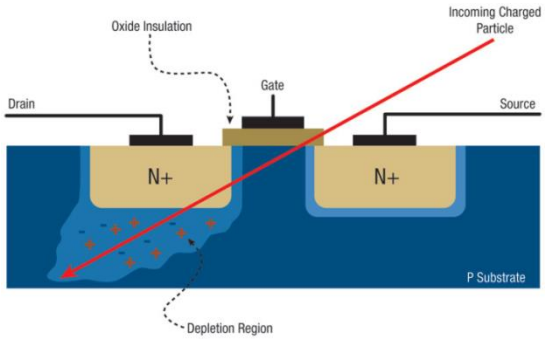
Capabilities Added to Charon to Support HBT Modeling

Sandia National Laboratories

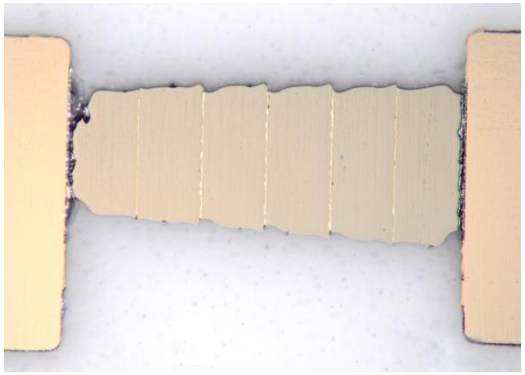
- Fermi-Dirac Statistics (highly doped)
- III-V Material Models
- Thermionic Emission
- Tunneling
- Recombination Terms
  - Direct
  - Auger
- Discontinuity of Concentrations at Heterojunction

Ongoing/Future Charon Development

- Expanding Physics Capability
  - SEE/SEU
    - Simple linear charge input available
  - Si HVD Analysis
  - GaN development
    - High Voltage Diodes (support of UWBG GC)
    - HEMTs
  - Frequency Domain Modeling (HB)
    - Both linear and non-linear
  - Improved coupled electrical & thermal
- Next Generation Development
  - In preparation of next gen computational Hardware

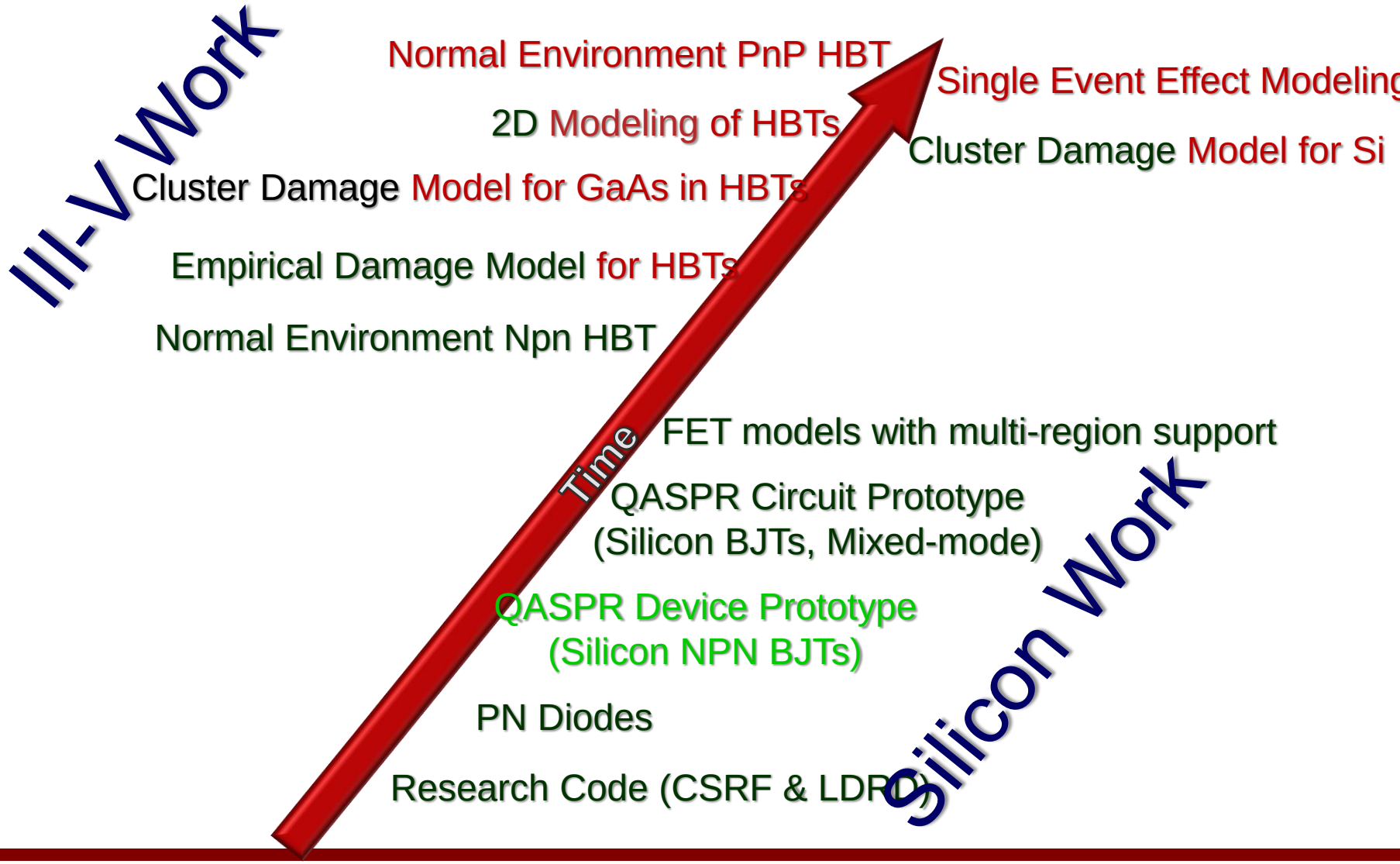


Single-Event Effects

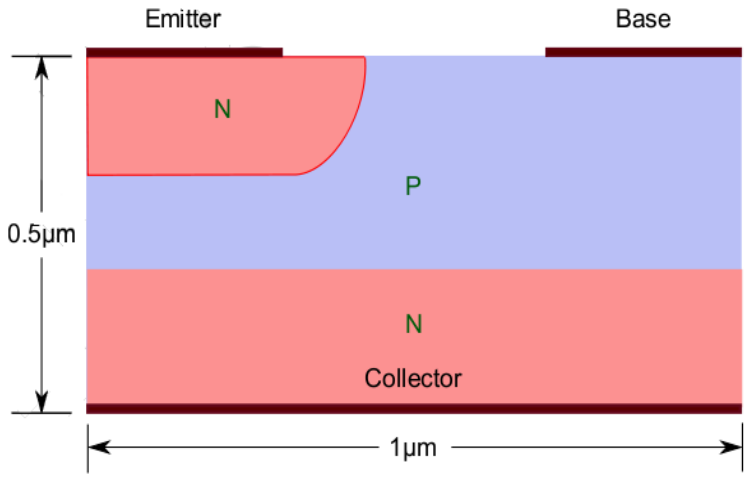


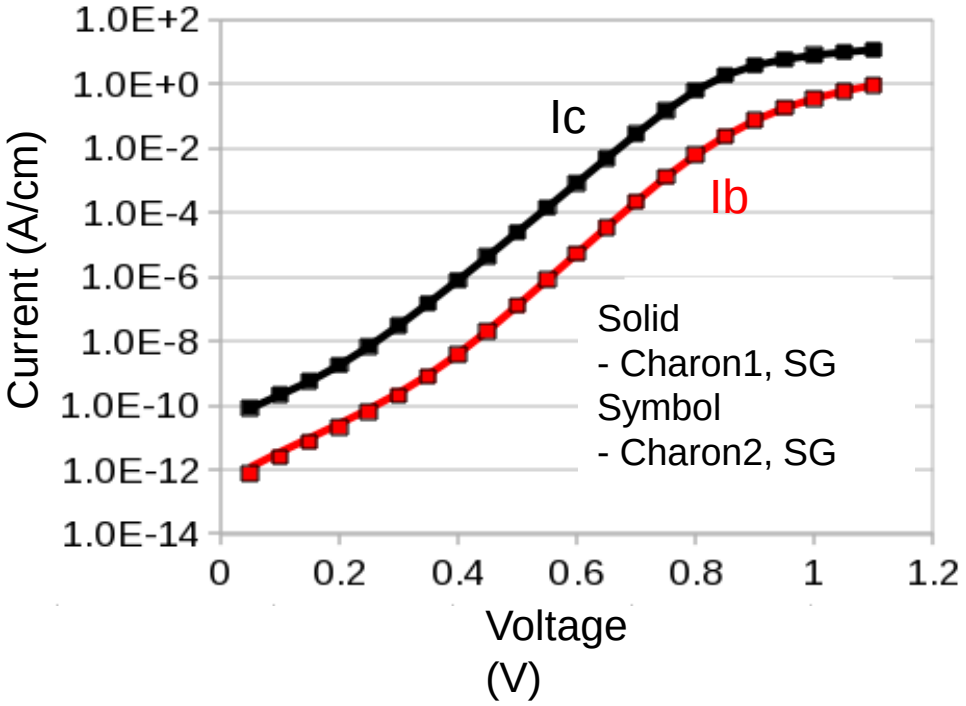
Cross section photo of High Voltage Diode (HVD)

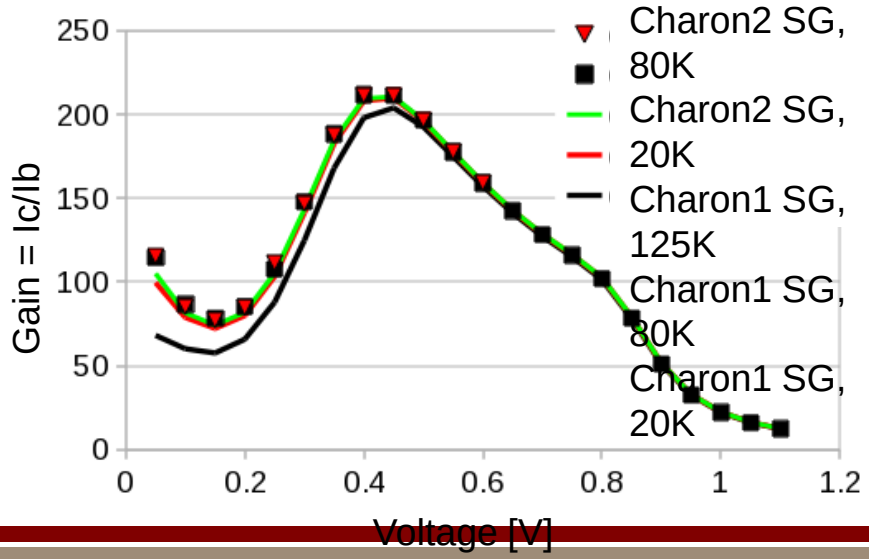
Progression of Charon Capabilities



Code Verification

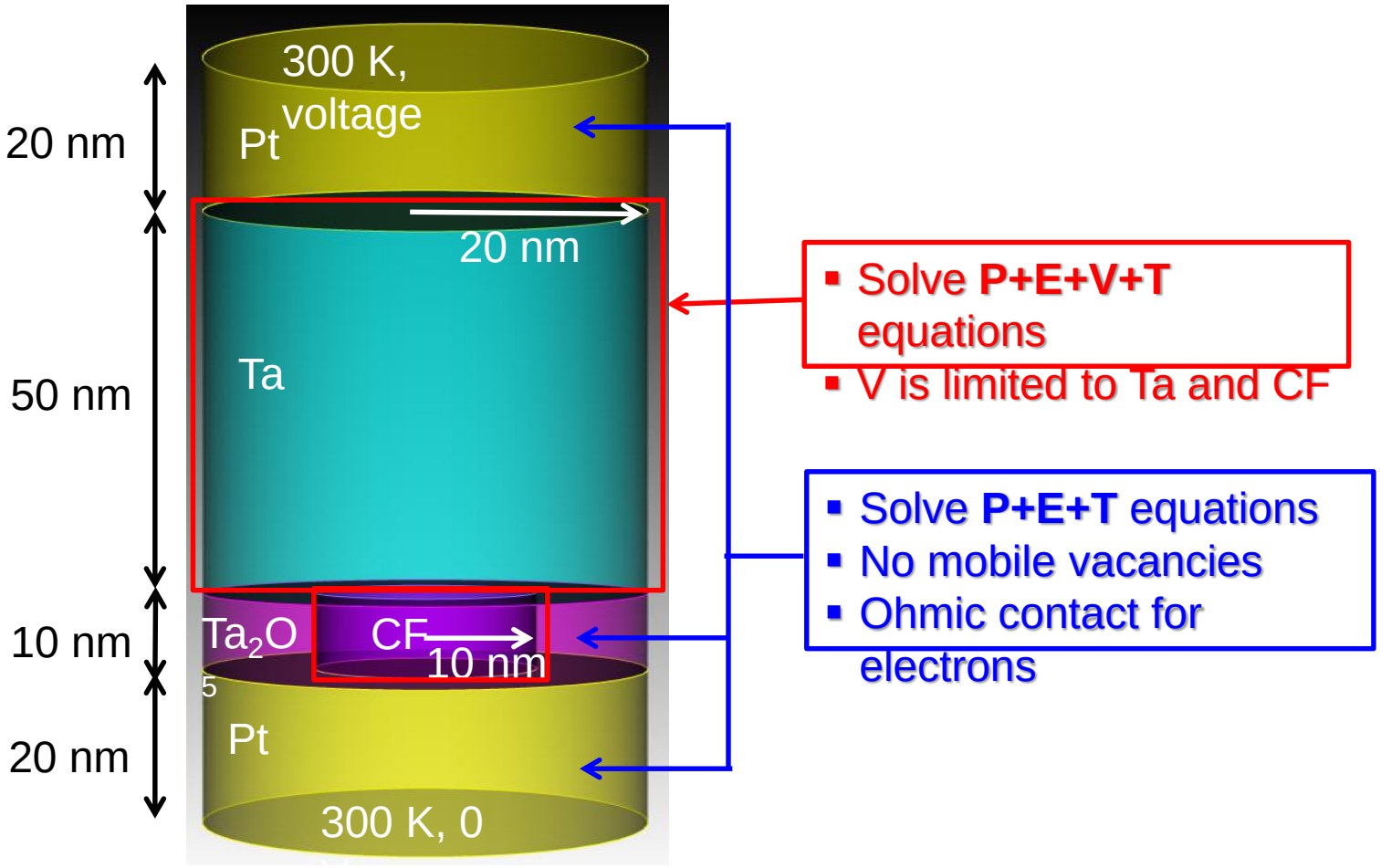






Charon1 SG shows strong mesh dependence of the gain when going from 20K to 80K quad elements, while Charon2 SG shows mesh convergence even for 20K elements !

TaOx Memristor Device Structure



Patrick R. Mickel et al., A physical model of switching dynamics in tantalum oxide memristive devices, APL **102**, 223502 (2013).

Charon Limitations

Sandia National Laboratories

- Not a commercial code
- Limited documentation
- Generally requires developer help
  - Non-intuitive input deck
    - A python interface is currently under development
- Different workflow from commercial codes
  - Cubit
  - Non-sequential input

Charon Availability

- No restrictions for Sandians
- Charon is categorized as an ITAR/Export Control Simulator
  - We have a Government Use Notice (GUN) in place with AWE
  - GUN provides a U.S. government agency or contractor access to software limited to government use
- Open-Source may be a future path
  - Currently in review